An International Journal
computers & mathematics with applications

PERGAMON Computers and Mathematics with Applications 39 (2000) 229–243
www.elsevier.nl/locate/camwa

Conservative Nonlinear Difference Scheme for the Cahn-Hilliard Equation—II

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Dedicated to Professor Tae-Geun Cho on the occasion of his 65th birthday

(Received and accepted November 1998)

Abstract—A nonlinear conservative difference scheme is considered for the two-dimensional Cahn-Hilliard equation. Existence of the solution for the finite difference scheme has been shown and the corresponding stability, convergence, and error estimates are discussed. We also show that the scheme preserves the discrete total mass computationally as well as analytically.

Keywords—Cahn-Hilliard equation, Conservation of mass, Nonlinear difference scheme.

1. INTRODUCTION

Consider the Cahn-Hilliard equation

$$u_t + \alpha\Delta^2 u = \Delta\phi(u), \qquad (x,y) \in \Omega, \quad 0 < t \le T, \tag{1.1a}$$

with boundary conditions

$$\frac{\partial u}{\partial \nu} = 0, \quad \frac{\partial}{\partial \nu}(\Delta u) = 0, \qquad (x,y) \in \partial\Omega, \quad 0 < t \le T, \tag{1.1b}$$

and an initial condition

$$u(x,y,0) = u_0(x,y), \qquad (x,y) \in \bar{\Omega}. \tag{1.1c}$$

Here $\phi(u) = \gamma(u^3 - \beta^2 u)$, and the constants α and γ are positive. The domain $\Omega = (0,l_1) \times (0,l_2)$ with its closure $\bar{\Omega}$ and boundary $\partial\Omega$.

The solution $u(x,y,t)$ is the difference of the respective concentrations of the two mixture components. The initial condition $u_0(x,y)$ is a given function. The operator $\Delta = \nabla^2$ is the Laplace operator and $\frac{\partial}{\partial \nu}$ is the outward normal derivative operator along the boundary $\partial\Omega$.

The Cahn-Hilliard equation (1.1) arises as a phenomenological continuum model for a phase separation. Immiscible binary mixtures such as Fe-Al alloys enjoy, under certain circumstances (cooling below a critical temperature), a phase separation phenomenon known as a spinodal decomposition. See [1] for a derivation of the model and [2] for more general models.

The authors would like to thank D. Greenspan for invaluable suggestions. SKC is supported in part by POSTECH under Grant BSRI-94-1430.

PII: S0898-1221(99)00326-0

Global existence and uniqueness of the solution for (1.1) have been shown by Elliot and Zheng [3] and Yin [4]. Long time behavior of the solution has been studied by Carr *et al.* [5] and Novick-Cohen and Segel [2].

Elliot and French [6] have studied phase separation of the classical solution for the one-dimensional Cahn-Hilliard equation with $u_0 \in H^2$ and verified those properties computationally. They used a finite element method and obtained an order of convergence $O(k^2 + h^2)$ which also depends on α^{-1}. This gives us a stringent condition to use the finite element method for small α.

For the two-dimensional problem, Elliot *et al.* [7] have shown that the weak solution of (1.1) satisfies conservation of mass and obtained optimal error bounds for the piecewise linear approximation using the splitting semidiscrete Galerkin method. They have shown existence of a Lyapunov functional, global existence of the solution, and conservation of mass. They have obtained order of convergence $O(h^2)$ analytically for a smooth initial data $u_0 \in H^1$. Elliot and Larsson [8] have also obtained optimal order of convergence for the problem with smooth and nonsmooth initial data without any computational results. Dean *et al.* [9] have shown existence of a mixed finite element approximation using the least squares method and checked spinodal decomposition of numerical solutions without any error analysis.

In spite of computational convenience of finite difference methods, there are few studies on finite difference methods compared to large amount of studies on finite element approximate solutions for (1.1) because of uneasy control of nonlinear terms in $\phi(u)$. In order to avoid this difficulty, Sun [10] has proposed a linearized difference scheme for (1.1) and obtained error estimates of second order under a smooth initial condition $u_0 \in C^4(\bar{\Omega})$. But the linearized scheme in [10] is only conditionally stable and does not preserve the total mass of mixtures. Choo and Chung [11] have applied a nonlinear conservative difference scheme based on the Crank-Nicolson scheme for a one-dimensional problem of the Cahn-Hilliard equation.

In this paper, we consider a nonlinear difference scheme for (1.1) which is unconditionally stable and conserves the total mass. This is an extension of Choo and Chung [11] to two-dimensional problems, which overcomes deficiency such as a severe restriction on α of [6] and nonconservation of total mass besides a smoothness condition of $u_0(x)$ in [10].

The outline of the paper is as follows. In Section 2, we analyze a nonlinear difference scheme for (1.1) and show that the scheme preserves the discrete total mass. In Section 3, we show existence and stability of the nonlinear scheme, which has a second-order accuracy. In Section 4, we give numerical examples which show the difference between the nonlinear difference scheme and the linearized scheme proposed by Sun [10], as well as the finite element method proposed by Dean *et al.* [9]. The nonlinear difference scheme preserves the discrete total mass besides giving physically meaningful numerical results for various initial conditions in either a spectral domain or a metastable domain.

2. NONLINEAR FINITE DIFFERENCE SCHEME

For the discretization of (1.1), let M_1, M_2, N be positive integers and $h_1 = l_1/M_1$, $h_2 = l_2/M_2$, $k = T/N$. Let $h = \max\{h_1, h_2\}$ and

$$\bar{\Omega}_h = \{(x_i, y_j) \mid x_i = ih_1,\ y_j = jh_2,\ 0 \le i \le M_1,\ 0 \le j \le M_2\}.$$

Let $w = (w_{ij})$ and $v = (v_{ij})$, $0 \le i \le M_1$, $0 \le j \le M_2$, are mesh functions defined on $\bar{\Omega}_h$. Denote

$$\begin{aligned}
D_x^+ w_{ij} &= \frac{w_{i+1,j} - w_{ij}}{h_1}, & D_x^- w_{ij} &= \frac{w_{ij} - w_{i-1,j}}{h_1}, \\
D_y^+ w_{ij} &= \frac{w_{i,j+1} - w_{ij}}{h_2}, & D_y^- w_{ij} &= \frac{w_{ij} - w_{i,j-1}}{h_2}, \\
D_x^2 &= D_x^+ D_x^-, & D_y^2 &= D_y^+ D_y^-, \\
D_x^4 &= D_x^2 D_x^2, & D_y^4 &= D_y^2 D_y^2 \\
\nabla_h^2 &= D_x^2 + D_y^2, & \nabla_h^4 &= \nabla_h^2 \nabla_h^2.
\end{aligned}$$

Define the discrete inner product and the discrete L_2-norm, respectively, by

$$(w,v)_h = \frac{h_1 h_2}{4}\sum_{i=1}^{M_1}\sum_{j=1}^{M_2}\left(w_{ij}v_{ij} + w_{i-1,j}v_{i-1,j} + w_{i,j-1}v_{i,j-1} + w_{i-1,j-1}v_{i-1,j-1}\right),$$

and

$$\|w\|_h = (w,w)_h^{1/2}.$$

If there is no confusion, $(\cdot,\cdot)$ and $\|\cdot\|$ will be used instead of $(\cdot,\cdot)_h$ and $\|\cdot\|_h$, respectively. The following identities can be shown by summation by parts.

LEMMA 2.1. *For functions v and w defined on $\bar{\Omega}_h$, we have*

(1) $(D_x^2 w, v) = -(1/2)(h_2)/(h_1)\sum_{j=1}^{M_2}\sum_{i=1}^{M_1}\{(w_{ij} - w_{i-1,j})(v_{ij} - v_{i-1,j}) + (w_{ij-1} - w_{i-1,j-1})(v_{ij-1} - v_{i-1,j-1})\}$;

(2) $(D_y^2 w, v) = -(1/2)(h_1)/(h_2)\sum_{i=1}^{M_1}\sum_{j=1}^{M_2}\{(w_{ij} - w_{i,j-1})(v_{ij} - v_{i,j-1}) + (w_{i-1,j} - w_{i-1,j-1})(v_{i-1,j} - v_{i-1,j-1})\}$;

(3) $(\nabla_h^2 w, v) = (w, \nabla_h^2 v)$;

(4) $(\nabla_h^4 w, v) = (\nabla_h^2 w, \nabla_h^2 v)$.

Denote $u_{ij}^n = u(x_i, y_j, t_n)$ with $t_n = nk$ and let

$$u_{ij}^{n+1/2} = \frac{u_{ij}^{n+1} + u_{ij}^n}{2}, \qquad \partial_t u_{ij}^n = \frac{u_{ij}^{n+1} - u_{ij}^n}{k}.$$

Then the approximate solution U_{ij}^n for (1.1) is defined as a solution of

$$\partial_t U_{ij}^m + \alpha\nabla_h^4 U_{ij}^{m+1/2} = \nabla_h^2\phi\left(U_{ij}^{m+1/2}\right), \tag{2.1a}$$

for $0 < i < M_1$, $0 < j < M_2$, $0 \le m \le N-1$ with boundary conditions

$$\begin{aligned}
D_x^2 U_{0j} &= \frac{2}{h_1}D_x^+ U_{0j}, & D_x^2 U_{M_1 j} &= -\frac{2}{h_1}D_x^- U_{M_1 j}, & 0 \le j \le M_2,\\
D_y^2 U_{i0} &= \frac{2}{h_2}D_y^+ U_{i0}, & D_y^2 U_{iM_2} &= -\frac{2}{h_2}D_y^- U_{iM_2}, & 0 \le i \le M_1,\\
D_x^4 U_{0j} &= \frac{2}{h_1}D_x^+ D_x^2 U_{0j}, & D_x^4 U_{M_1 j} &= -\frac{2}{h_1}D_x^- D_x^2 U_{M_1 j}, & 0 \le j \le M_2,\\
D_y^4 U_{i0} &= \frac{2}{h_2}D_y^+ D_y^2 U_{i0}, & D_y^4 U_{iM_2} &= -\frac{2}{h_2}D_y^- D_y^2 U_{iM_2}, & 0 \le i \le M_1,
\end{aligned} \tag{2.1b}$$

and an initial condition

$$U_{ij}^0 = u_0(x_i, y_j). \tag{2.1c}$$

It is well known that for the solution u of the Cahn-Hilliard equation (1.1), the property of mass conservation holds;

$$\iint_\Omega u(x,y,t)\,dx\,dy = \text{constant}, \qquad 0 \le t \le T. \tag{2.2}$$

As in the continuous case, the property of mass conservation holds when the finite difference scheme (2.1) is applied together with the trapezoidal rule for an approximation of the integral (2.2).

THEOREM 2.1. *For the solution U^m of (2.1), the property of mass conservation holds; for any $0 \le m \le N$,*

$$\frac{h_1 h_2}{4}\sum_{i=1}^{M_1}\sum_{j=1}^{M_2}\left(U_{ij}^m + U_{i-1,j}^m + U_{i,j-1}^m + U_{i-1,j-1}^m\right) = \frac{h_1 h_2}{4}\sum_{i=1}^{M_1}\sum_{j=1}^{M_2}\left(U_{ij}^0 + U_{i-1,j}^0 + U_{i,j-1}^0 + U_{i-1,j-1}^0\right).$$

PROOF. It follows from (2.1) that

$$\partial_t \left[\frac{h_1 h_2}{4} \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} \left(U_{ij}^m + U_{i-1,j}^m + U_{i,j-1}^m + U_{i-1,j-1}^m \right) \right]$$

$$= h_1 h_2 \left[\sum_{i=1}^{M_1-1} \sum_{j=1}^{M_2-1} \nabla_h^2 \phi \left(U_{ij}^{m+1/2} \right) + \frac{1}{2} \sum_{i=1}^{M_1-1} \nabla_h^2 \left\{ \phi \left(U_{i0}^{m+1/2} \right) + \phi \left(U_{iM_2}^{m+1/2} \right) \right\} \right.$$

$$+ \frac{1}{2} \sum_{j=1}^{M_2-1} \nabla_h^2 \left\{ \phi \left(U_{0j}^{m+1/2} \right) + \phi \left(U_{M_1 j}^{m+1/2} \right) \right\}$$

$$\left. + \frac{1}{4} \nabla_h^2 \left\{ \phi \left(U_{00}^{m+1/2} \right) + \phi \left(U_{M_1 0}^{m+1/2} \right) + \phi \left(U_{0M_2}^{m+1/2} \right) + \phi \left(U_{M_1 M_2}^{m+1/2} \right) \right\} \right]$$

$$- h_1 h_2 \left[\sum_{i=1}^{M_1-1} \sum_{j=1}^{M_2-1} \nabla_h^2 \left(\nabla_h^2 U_{ij}^{m+1/2} \right) + \frac{1}{2} \sum_{i=1}^{M_1-1} \nabla_h^2 \left(\nabla_h^2 U_{i0}^{m+1/2} + \nabla_h^2 U_{iM_2}^{m+1/2} \right) \right.$$

$$+ \frac{1}{2} \sum_{j=1}^{M_2-1} \nabla_h^2 \left(\nabla_h^2 U_{0j}^{m+1/2} + \nabla_h^2 U_{M_1 j}^{m+1/2} \right)$$

$$\left. + \frac{1}{4} \nabla_h^2 \left(\nabla_h^2 U_{00}^{m+1/2} + \nabla_h^2 U_{M_1 0}^{m+1/2} + \nabla_h^2 U_{0M_2}^{m+1/2} + \nabla_h^2 U_{M_1 M_2}^{m+1/2} \right) \right].$$

Applying the boundary conditions, we obtain

$$\partial_t \left[\frac{h_1 h_2}{4} \sum_{i=1}^{M_1} \sum_{j=1}^{M_2} \left(U_{ij}^m + U_{i-1,j}^m + U_{i,j-1}^m + U_{i-1,j-1}^m \right) \right] = 0.$$

Summation in time completes the proof. ∎

3. EXISTENCE AND CONVERGENCE

In this section, existence and stability of the solution are shown for the difference scheme (2.1). Error estimates for (2.1) is obtained, which show the finite difference scheme is of a second-order convergence.

LEMMA 3.1. *Let $U = U^m$ be a solution of (2.1) defined on $\bar{\Omega}_h$. Then*

$$- \left(\nabla_h^2 \phi(U), U \right) \geq \gamma \beta^2 \left(\nabla_h^2 U, U \right).$$

PROOF. It follows from Lemma 2.1 and direct summation that

$$- \left(D_x^2 \phi(U), U \right) = -\gamma \left(D_x^2 U^3, U \right) + \gamma \beta^2 \left(D_x^2 U, U \right)$$

$$= \frac{\gamma}{2} \frac{h_2}{h_1} \left[\sum_{j=1}^{M_2} \sum_{i=1}^{M_1} \left(U_{ij}^3 - U_{i-1,j}^3 \right) \left(U_{ij} - U_{i-1,j} \right) \right.$$

$$\left. + \sum_{j=1}^{M_2} \sum_{i=1}^{M_1} \left(U_{i,j-1}^3 - U_{i-1,j-1}^3 \right) \left(U_{i,j-1} - U_{i-1,j-1} \right) \right] + \gamma \beta^2 \left(D_x^2 U, U \right)$$

$$= \frac{\gamma}{2} \frac{h_2}{h_1} \left[\sum_{j=1}^{M_2} \sum_{i=1}^{M_1} \left(U_{ij}^2 + U_{ij} U_{i-1,j} + U_{i-1,j}^2 \right) \left(U_{ij} - U_{i-1,j} \right)^2 \right.$$

$$
\left. + \sum_{j=1}^{M_2} \sum_{i=1}^{M_1} \left(U_{i,j-1}^2 + U_{i,j-1}U_{i-1,j-1} + U_{i-1,j-1}^2\right)\left(U_{i,j-1} - U_{i-1,j-1}\right)^2 \right]
$$
$$
+ \gamma\beta^2 \left(D_x^2 U, U\right)
$$
$$
\geq \gamma\beta^2 \left(D_x^2 U, U\right).
$$

Similarly, we obtain

$$
-\left(D_y^2 \phi(U), U\right) \geq \gamma\beta^2 \left(D_y^2 U, U\right).
$$

These complete the proof. ∎

We now prove the existence of solutions for (2.1) using the Brouwer fixed-point theorem.

THEOREM 3.1. *The solution U^n of the finite difference scheme (2.1) exists.*

PROOF. In order to prove the theorem by the induction, assume that $U^0, U^1, \dots, U^n$ exist for $n < N$. Let $g : \bar{\Omega}_h \to \mathbb{R}$ be a function defined by

$$
g(V) = 2V - 2U^n + k\alpha\nabla_h^4 V - k\nabla_h^2\phi(V).
$$

Then g is clearly continuous. Taking an inner product of $g(V)$ with V and using Young's inequality, it follows from Lemma 2.1 and Lemma 3.1 that

$$
\begin{aligned}
(g(V), V) &= 2(V, V) - 2\left(U^n, V\right) + k\alpha\left(\nabla_h^4 V, V\right) - k\left(\nabla_h^2\phi(V), V\right) \\
&\geq 2\|V\|^2 - 2\left\|U^n\right\|\|V\| + k\alpha\left\|\nabla_h^2 V\right\|^2 - k\gamma\beta^2\left\|\nabla_h^2 V\right\|\|V\| \\
&\geq 2\|V\|^2 - \left\{\left\|U^n\right\|^2 + \|V\|^2\right\} + k\alpha\left\|\nabla_h^2 V\right\|^2 - \left\{k\alpha\left\|\nabla_h^2 V\right\|^2 + \frac{k}{4\alpha}\left(\gamma\beta^2\right)^2\|V\|^2\right\} \\
&\geq \left\{1 - \frac{k}{4\alpha}\left(\gamma\beta^2\right)^2\right\}\|V\|^2 - \left\|U^n\right\|^2.
\end{aligned}
$$

If we take k such that $k < 4\alpha/(\gamma\beta^2)^2$, then $(g(V), V) \geq 0$ for all V such that $\|V\| = \|U^n\|/(1 - (k/4\alpha)(\gamma\beta^2)^2)$. The Brouwer fixed-point theorem implies the existence of the solution of $g(V) = 0$. We complete the proof by taking $U^{n+1} = 2V - U^n$. ∎

We now show that the scheme (2.1) is unconditionally stable.

THEOREM 3.2. *Let U^n be the solution of (2.1). Then there exists a constant C such that*

$$
\left\|U^n\right\| \leq C\left\|U^0\right\|, \qquad 1 \leq n \leq N.
$$

PROOF. Forming an inner product between (2.1) and $U^{m+1/2}$, we obtain

$$
\left(\partial_t U^m, U^{m+1/2}\right) + \alpha\left(\nabla_h^4 U^{m+1/2}, U^{m+1/2}\right) = \left(\nabla_h^2\phi\left(U^{m+1/2}\right), U^{m+1/2}\right).
$$

It follows from Lemma 3.1 and Young's inequality that

$$
\begin{aligned}
\frac{1}{2}\partial_t\left\|U^m\right\|^2 + \alpha\left\|\nabla_h^2 U^{m+1/2}\right\|^2 &\leq -\gamma\beta^2\left(\nabla_h^2 U^{m+1/2}, U^{m+1/2}\right) \\
&\leq \alpha\left\|\nabla_h^2 U^{m+1/2}\right\|^2 + \frac{1}{4\alpha}\left(\gamma\beta^2\right)^2\left\|U^{m+1/2}\right\|^2.
\end{aligned}
$$

Hence,

$$
\partial_t\left\|U^m\right\|^2 \leq \frac{1}{4\alpha}\left(\gamma\beta^2\right)^2\left(\left\|U^{m+1}\right\|^2 + \left\|U^m\right\|^2\right).
$$

Summing from $m = 0$ to $m = n - 1$, we obtain

$$
\left\{1 - k\frac{\left(\gamma\beta^2\right)^2}{4\alpha}\right\}\left\|U^n\right\|^2 \leq \left\|U^0\right\|^2 + \frac{\left(\gamma\beta^2\right)^2}{2\alpha}k\sum_{m=0}^{n-1}\left\|U^m\right\|^2.
$$

Applying the discrete Gronwall's inequality with sufficiently small k such that $1 - k((\gamma\beta^2)^2/4\alpha) > 0$, we obtain the desired result. ∎

Let u^n and U^n be solutions for (1.1) and (2.1), respectively, and $e^n = u^n - U^n$. Then the following error estimate is obtained.

THEOREM 3.3. *If $\|U^n\|_\infty$ and $\|u^n\|_\infty$ are bounded, then there exists a constant C such that*

$$\|e^n\| \le C\left(k^2 + h^2\right).$$

PROOF. Replacing U^m by $u^m - e^m$ in (2.1), we obtain that

$$\begin{aligned}
\partial_t e^m + \alpha\nabla_h^4 e^{m+1/2} &= \partial_t u^m + \alpha\nabla_h^4 u^{m+1/2} - \nabla_h^2\phi\left(U^{m+1/2}\right) \\
&= u_t\left(t_{m+1/2}\right) + \Delta^2 u\left(t_{m+1/2}\right) - \nabla_h^2\phi\left(U^{m+1/2}\right) + O\left(h^2 + k^2\right) \\
&= \Delta\phi\left(u^{m+1/2}\right) - \nabla_h^2\phi\left(U^{m+1/2}\right) + O\left(h^2 + k^2\right) \\
&= \nabla_h^2\phi\left(u^{m+1/2}\right) - \nabla_h^2\phi\left(U^{m+1/2}\right) + O\left(h^2 + k^2\right).
\end{aligned}$$

Forming the inner product with $e^{m+1/2}$, applying Lemma 2.1 and Young's inequality, we obtain

$$\begin{aligned}
&\frac{1}{2}\partial_t \|e^m\|^2 + \alpha\left\|\nabla_h^2 e^{m+1/2}\right\|^2 \\
&\quad\le \gamma\left(\nabla_h^2\left(u^{m+1/2}\right)^3 - \nabla_h^2\left(U^{m+1/2}\right)^3, e^{m+1/2}\right) - \gamma\beta^2\left(\nabla_h^2 e^{m+1/2}, e^{m+1/2}\right) \\
&\qquad + \left\|e^{m+1/2}\right\|^2 + O\left(h^4 + k^4\right) \\
&\quad\le \gamma\left(\left[\left(u^{m+1/2}\right)^2 + u^{m+1/2}U^{m+1/2} + \left(U^{m+1/2}\right)^2\right] e^{m+1/2}, \nabla_h^2 e^{m+1/2}\right) \\
&\qquad - \gamma\beta^2\left(\nabla_h^2 e^{m+1/2}, e^{m+1/2}\right) + \left\|e^{m+1/2}\right\|^2 + O\left(h^4 + k^4\right).
\end{aligned}$$

Since $\|u^n\|_\infty$ and $\|U^n\|_\infty$ are bounded, there exists a constant C_1 such that

$$\partial_t \|e^m\|^2 \le C_1\left\|e^{m+1/2}\right\|^2 + C_1\left(h^4 + k^4\right).$$

Summing from $m = 0$ to $n - 1$, we obtain

$$\left(1 - \frac{k}{2}C_1\right)\|e^n\|^2 \le C_1\left(h^4 + k^4\right) + C_2 k\sum_{m=0}^{n-1}\|e^m\|^2.$$

Applying the discrete Gronwall's inequality with small k such that $1 - (k/2)C_1 > 0$, we obtain the desired result. ∎

4. NUMERICAL EXAMPLES

In this section, we show that the total mass is conserved by the nonlinear finite difference scheme (2.1). We compare the nonlinear difference scheme (2.1) with the linearized difference scheme proposed by Sun [10] and the finite element method proposed by Dean *et al.* [9].

First, the linearized difference scheme proposed by Sun [10] follows as: for $0 \le i \le M_1$, $0 \le j \le M_2$, $m \ge 1$,

$$\frac{U_{ij}^{m+1} - U_{ij}^{m-1}}{2k} + \alpha\nabla^4\frac{U_{ij}^{m+1} + U_{ij}^{m-1}}{2} = \nabla^2\phi\left(U_{ij}^m\right), \tag{4.1a}$$

with boundary conditions (2.1b) and initial conditions

$$U_{ij}^0 = u_0(x_i, y_j), \qquad U_{ij}^1 = u_0(x_i, y_j) + k\Delta \{\phi(u_0(x_i, y_j)) - \Delta u_0(x_i, y_j)\}. \tag{4.1b}$$

Because of (4.1b), the linearized scheme (4.1) can be only applied to the Cahn-Hilliard equation with a smooth initial condition. It is shown in [10] that the scheme (4.1) is conditionally stable and convergent of order $O(h^2 + k^2)$.

In the following numerical examples, we consider the Cahn-Hilliard equation with a domain $\Omega = (0,1) \times (0,1)$, $T = 0.5$, $\alpha = 0.01$, and $\gamma = \beta = 1$. Since $\phi(u) = u^3 - u$, the interval $[-1/\sqrt{3},\ 1/\sqrt{3}]$ becomes the spinodal domain and intervals $(-1, -1/\sqrt{3})$ and $(1/\sqrt{3}, 1)$ become metastable domains.

Let $Q : R^{(M_1+1)\cdot(M_2+1)} \to R^{(M_1+1)\cdot(M_2+1)}$ be a function with components q_{ij} such that

$$q_{ij}\left(U_{00}^n, U_{10}^n, \dots, U_{ij}^n, \dots, U_{M_1M_2}^n\right) = \frac{U_{ij}^n - U_{ij}^n}{2k} + \alpha\nabla^4 \frac{U_{ij}^n + U_{ij}^n}{2} - \nabla^2\phi\left(\frac{U_{ij}^n + U_{ij}^n}{2}\right).$$

In order to obtain computational solutions, we have to solve a system of difference equations of the type

$$q_{ij}\left(U_{00}^n, U_{10}^n, \dots, U_{ij}^n, \dots, U_{M_1M_2}^n\right) = 0$$

obtained from a system of nonlinear difference equation (2.1) and a system of linear difference equation for (4.1). We use the generalized Newton's method

$$U_{ij}^{n,(l+1)} = U_{ij}^{n,(l)} - \omega \frac{q_{ij}\left(U_{00}^{n,(l+1)}, \dots, U_{(i-1)j}^{n,(l+1)}, U_{ij}^{n,(l)}, \dots, U_{M_1M_2}^{n,(l)}\right)}{\dfrac{\partial q_{ij}\left(U_{00}^{n,(l+1)}, \dots, U_{(i-1)j}^{n,(l+1)}, U_{ij}^{n,(l)}, \dots, U_{M_1M_2}^{n,(l)}\right)}{\partial U_{ij}^n}}.$$

For the computational results, we use step sizes in spatial direction $h = h_1 = h_2 = 0.1$ ($M_1 = M_2 = 10$) and in temporal direction $k = 0.01$ with relaxation parameter $\omega = 0.3$ for both (2.1) and (4.1). We stop the numerical computations when the relative error between l^{th}- and $(l+1)^{\text{th}}$-iterations become less than 10^{-7}. That is,

$$\frac{\left|U_{ij}^{n,(l+1)} - U_{ij}^{n,(l)}\right|}{\left|U_{ij}^{n,(l)}\right|} \le 10^{-7}.$$

For the numerical computation of total mass, we approximate the integral

$$\int_0^1 \int_0^1 u(x, y, t_n)\, dx\, dy$$

by the quadrature rule

$$f(n) = \frac{h^2}{4} \sum_{j=1}^{M_1} \sum_{i=1}^{M_2} \left\{U_{ij}^n + U_{i-1,j}^n + U_{i,j-1}^n + U_{i-1,j-1}^n\right\}.$$

EXAMPLE 4.1. THE PEAK INITIAL DATA IN THE SPINODAL DOMAIN. Consider the Cahn-Hilliard equation with an initial condition

$$u_0(x, y) = 0.1 + 0.4\phi_{i_0,j_0},$$

where ϕ_{i_0,j_0} is a basis function of H_h^1 associated to the vertex (i_0, j_0) of the rectangulation of Ω; for $i_0 = j_0 = 6$

$$\phi_{i_0,j_0}(ih, jh) = \begin{cases} 1.0, & \text{if } (i,j) = (i_0, j_0), \\ 0.0, & \text{if } (i,j) \ne (i_0, j_0). \end{cases}$$

Figures 1–3 show the numerical solutions at $t = 0.0, 0.1, 0.5$, respectively. We can see the spinodal decomposition when the initial data are in the spinodal domain. Figure 4 shows the approximate total mass $f(n)$ obtained by the scheme (2.1) at $t = 10^{-2}n$. This indicates that the scheme (2.1) preserves the discrete total mass of initial data.

EXAMPLE 4.2. THE RANDOM INITIAL DATA IN THE SPINODAL DOMAIN. Consider the Cahn-Hilliard equation (1.1) with an initial condition

$$u_0(x,y) = 0.0001 + \sum_{0\le i,j\le 10} \Theta_{i,j}\phi_{i,j}(x,y),$$

where $\phi_{i,j}$ is a basis function of H_h^1 associated with the vertex (i,j) of the rectangulation of Ω and $\Theta_{i,j}$ is a random variable distributed over an interval $(-1,1)$.

Figures 5–7 show the numerical solutions at $t = 0.0, 0.1, 0.5$, respectively. We can also see the spinodal decomposition when the random initial data are in spinodal domain. Figure 8 displays the approximate total mass $f(n)$ obtained by scheme (2.1) at $t = 10^{-2}n$. This shows that the nonlinear difference scheme (2.1) preserves the discrete total mass of initial data.

EXAMPLE 4.3. THE INITIAL DATA IN THE METASTABLE DOMAIN. Consider the Cahn-Hilliard equation with an initial condition

$$u_0(x,y) = 0.3\cos(5x)\cos(5y)e^{-(5/4)\sqrt{x^2+y^2}} + 0.8,$$

where the mean value M of $u_0(x,y)$ is in the metastable region $(1/\sqrt{3}, 1)$.

Figures 9–11 show the numerical solutions at $t = 0.0, 0.1, 0.5$, respectively. Since the initial condition is in the metastable interval $(1/\sqrt{3}, 1)$, the numerical solution converges to M as we expect in [3]. Figure 12 shows the approximate total mass $f(n)$ obtained by scheme (2.1) at $t = 10^{-2}n$.

EXAMPLE 4.4. THE COMPARISON OF LINEARIZED SCHEME WITH THE NONLINEAR SCHEME. The linearized scheme (4.1) proposed by Sun [10] can be only applied to the physical problem having smooth initial data. For the comparison of the nonlinear difference scheme (2.1) with the linearized scheme (4.1), we consider the Cahn-Hilliard equation with a smooth initial condition

$$u_0(x,y) = 0.001x^4y^4(1-x)^4(1-y)^4. \tag{4.2}$$

Figure 13 shows the approximate total mass obtained by scheme (2.1) and (4.1). In the figure, the point • denotes the discrete mass of initial data (4.2). We can see that the nonlinear difference scheme (2.1) preserves the discrete mass of initial data, but the linearized difference scheme (4.1) does not.

As we can see in Figure 13, the total mass obtained by the linearized scheme (4.1) is alternating. This can be shown by following the idea in Theorem 2.1. In fact, the total mass obtained by the linearized scheme (4.1) appears alternately as, for $1 \le n \le N-1$,

$$\frac{h_1h_2}{4}\sum_{i=1}^{M_1}\sum_{j=1}^{M_2}\left(U_{ij}^{n+1} + U_{i-1,j}^{n+1} + U_{i,j-1}^{n+1} + U_{i-1,j-1}^{n+1}\right)$$
$$= \frac{h_1h_2}{4}\sum_{i=1}^{M_1}\sum_{j=1}^{M_2}\left(U_{ij}^{n-1} + U_{i-1,j}^{n-1} + U_{i,j-1}^{n-1} + U_{i-1,j-1}^{n-1}\right).$$

EXAMPLE 4.5. THE COMPARISON OF FINITE ELEMENT SCHEME WITH THE NONLINEAR SCHEME. In order to obtain numerical solutions of the Cahn-Hilliard problem (1.1), Dean *et al.* [9] have proposed the following fourth-order linearized method: for $n \ge 2$,

$$\frac{(3/2)u^{n+1} - 2u^n + (1/2)u^{n-1}}{k} - \nabla\cdot\left[3\left(2u^n - u^{n-1}\right)^2 - 1\right]\nabla u^{n+1} + \alpha\Delta^2 u^{n+1} = 0, \tag{4.3a}$$

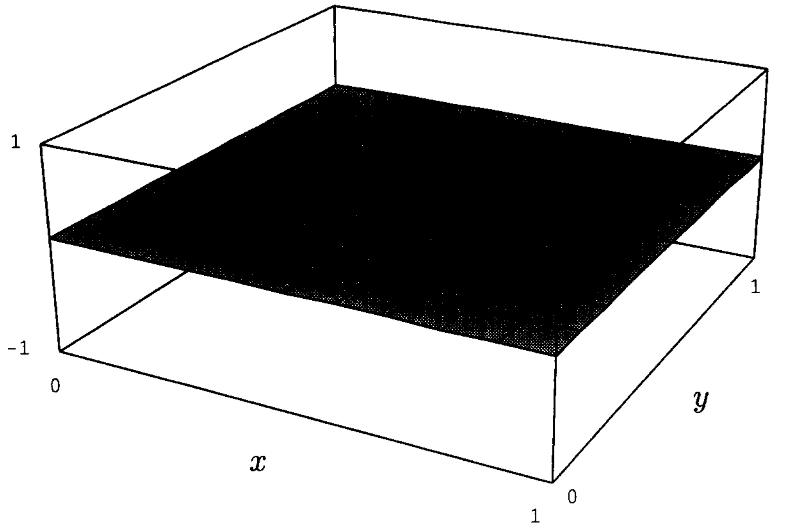

Figure 1. U^n at $t = 0$.

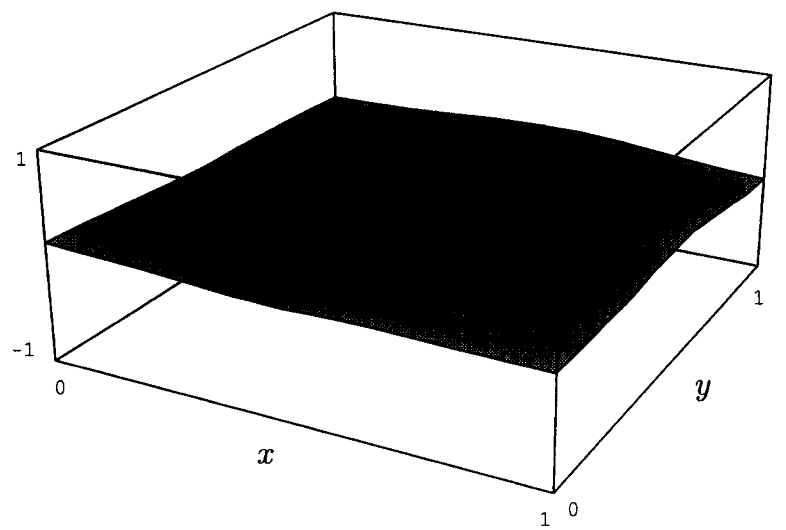

Figure 2. U^n at $t = 0.1$.

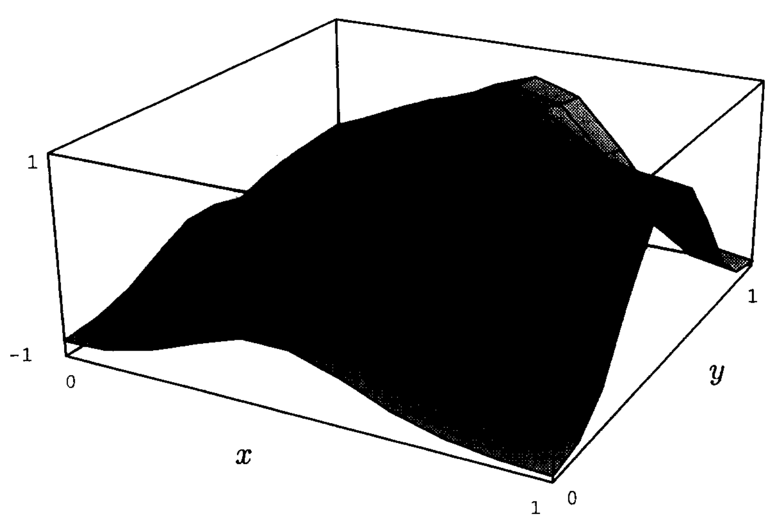

Figure 3. U^n at $t = 0.5$.

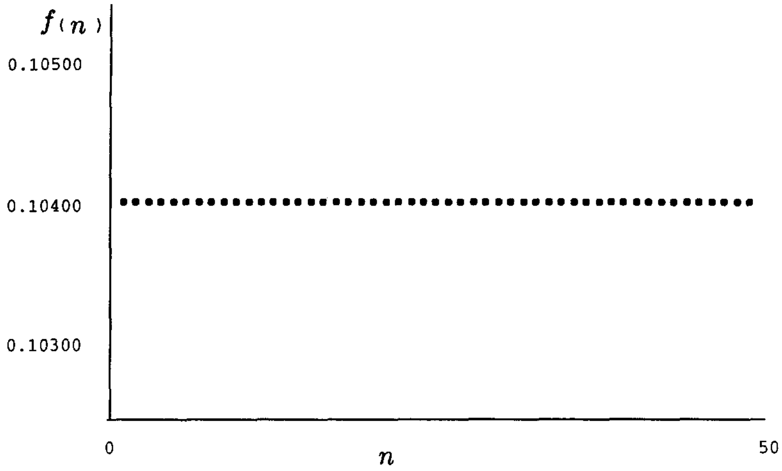

Figure 4. Total mass $f(n)$.

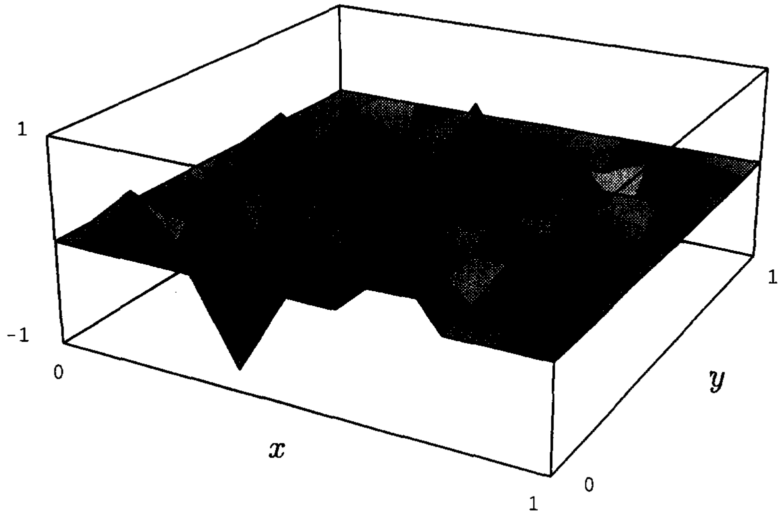

Figure 5. U^n at $t = 0$.

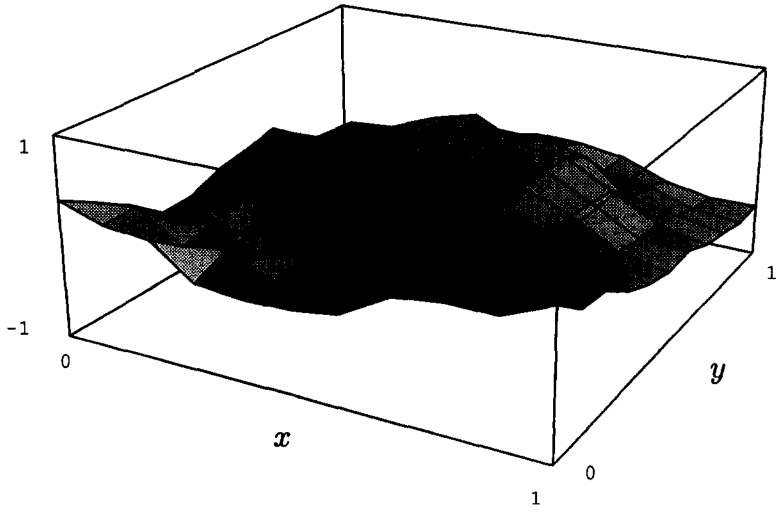

Figure 6. U^n at $t = 0.1$.

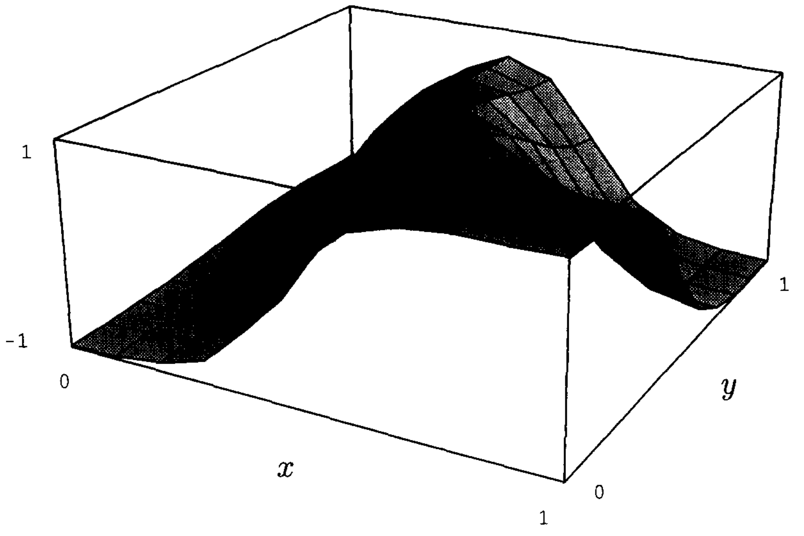

Figure 7. U^n at $t = 0.5$.

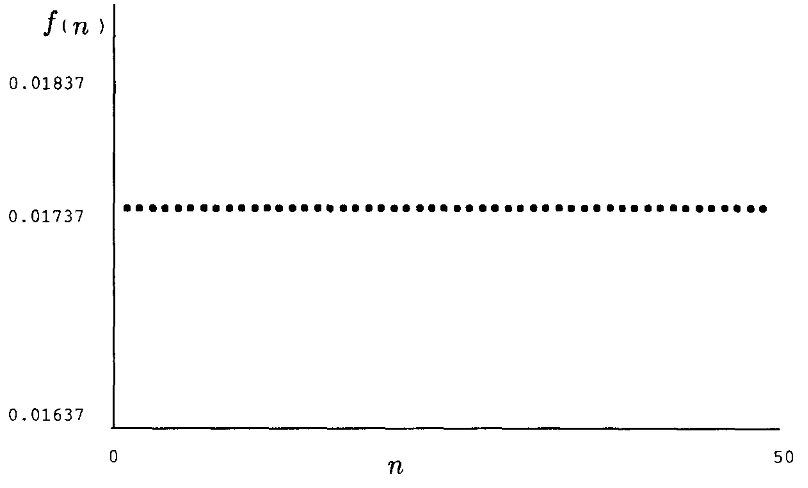

Figure 8. Total mass $f(n)$.

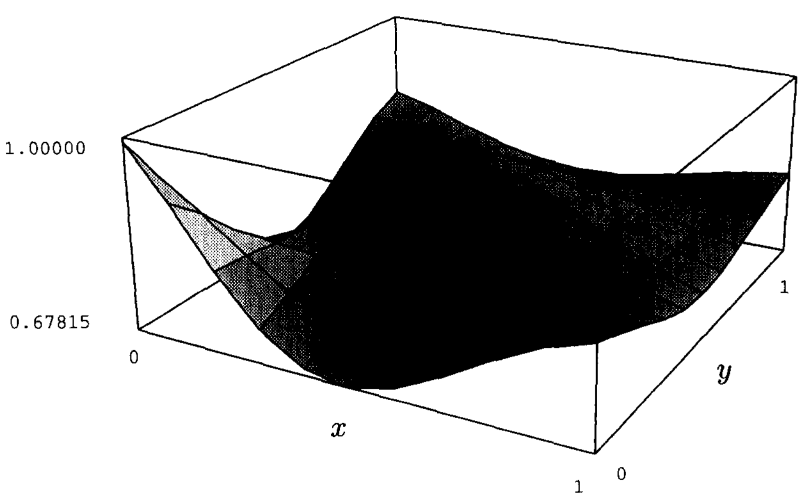

Figure 9. U^n at $t = 0$.

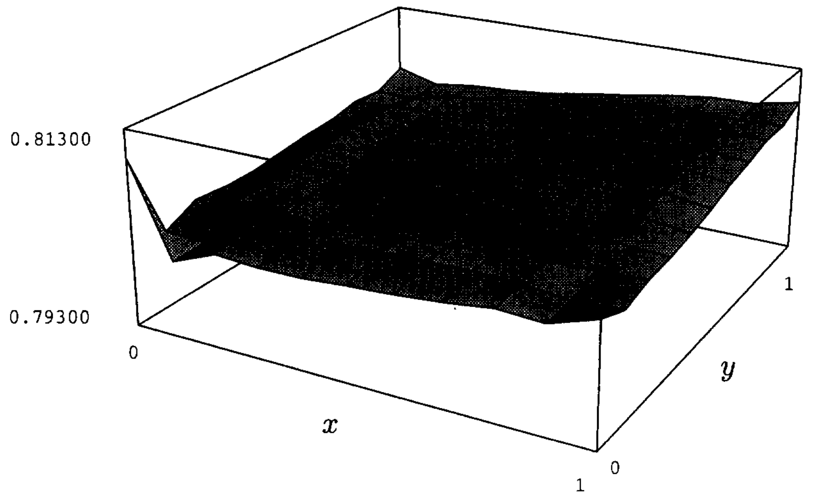

Figure 10. U^n at $t = 0.1$.

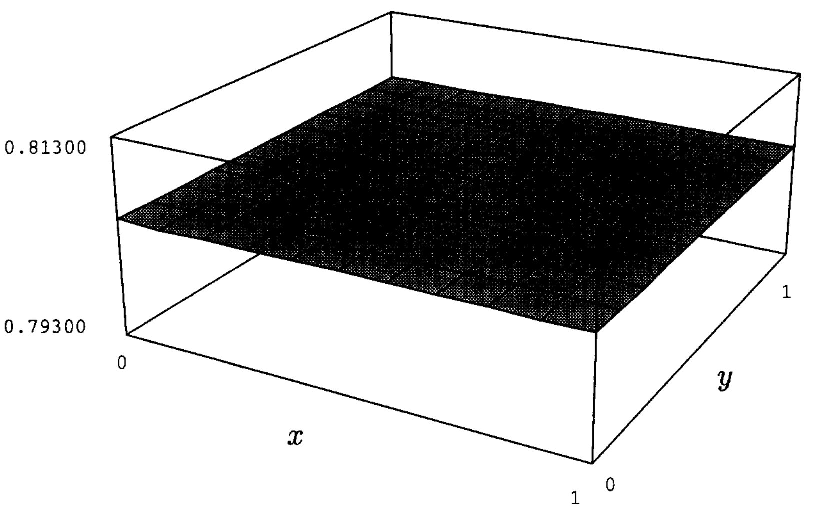

Figure 11. U^n at $t = 0.5$.

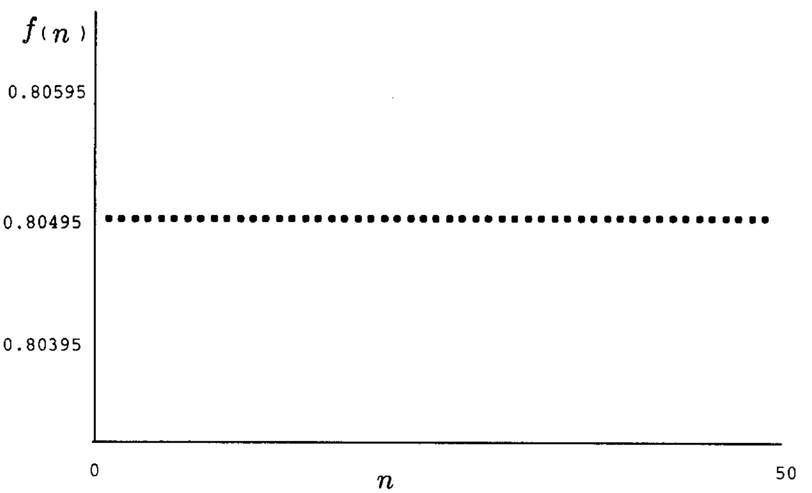

Figure 12. Total mass $f(n)$.

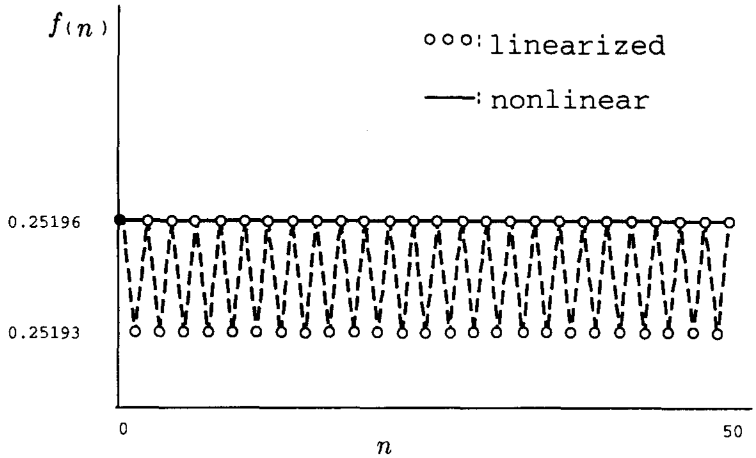

Figure 13. Total mass at $t = 10^{-2}n$.

$$\frac{u^1 - u_0}{k} - \nabla \cdot \left(3u_0^2 - 1\right) \nabla u^1 + \alpha \Delta^2 u^1 = 0, \tag{4.3b}$$

$$\frac{\partial u^1}{\partial \nu} = \frac{\partial \Delta u^1}{\partial \nu} = 0. \tag{4.3c}$$

Because of the biharmonic term in (4.3), (4.3) needs a finite-dimensional subspace spanned by piecewise polynomials of degree not less than 2 in order to obtain numerical solution by finite element methods. In order to reduce higher regularity of the bases functions, they split the equation and derive a system of coupled second-order elliptic equations from (4.3). They obtain a numerical solution u^{n+1} in the space H_h^1.

For the comparison of numerical solutions obtained from the finite element method (4.3) with the nonlinear scheme (2.1), we consider equation (1.1) with an initial condition $u_0(x, y)$ as in Example 4.1. Figures 14–16 show numerical solutions at $t = 0.1, 0.5, 5.0$, respectively. We can see the spinodal decomposition when the initial data are in the spinodal domain. Figure 17 shows the total mass $f(t_n)$ obtained by the finite element method (4.3) at $t = 10^{-2}n$. This indicates that the method (4.3) preserves the total mass of initial data. In fact, we may show theoretically that the finite element method (4.3) preserves the total mass.

Table 1 shows that the difference between numerical solutions obtained by the nonlinear conservative scheme (2.1) and those obtained by the finite element method (4.3) using the temporal step size $k = 1/100$. In the table, Max $= \max_{x_n} |U_{\mathrm{FDM}}(x_n, t) - U_{\mathrm{FEM}}(x_n, t)|$ and $L_2 = \|U_{\mathrm{FDM}}(t) - U_{\mathrm{FEM}}(t)\|$, where U_{FDM} and U_{FEM} mean numerical solutions obtained by the nonlinear conservative method (2.1) and the finite element method (4.3), respectively. We may find that numerical results obtained by (2.1) and (4.3) are in good agreement and that the observed differences can be related to the order of accuracy of the step sizes.

Table 4.1. Numerical comparison of FDM with FEM.

h	t	Max	L_2
$\frac{1}{10}$	0.5	0.253	0.102
	5.0	0.177	0.050
$\frac{1}{20}$	0.5	0.024	0.011
	5.0	0.048	0.014

5. CONCLUDING REMARKS

A conservative nonlinear difference scheme for the two-dimensional Cahn-Hilliard equation is considered based on the Crank-Nicolson scheme. This is an extension of the previous work done

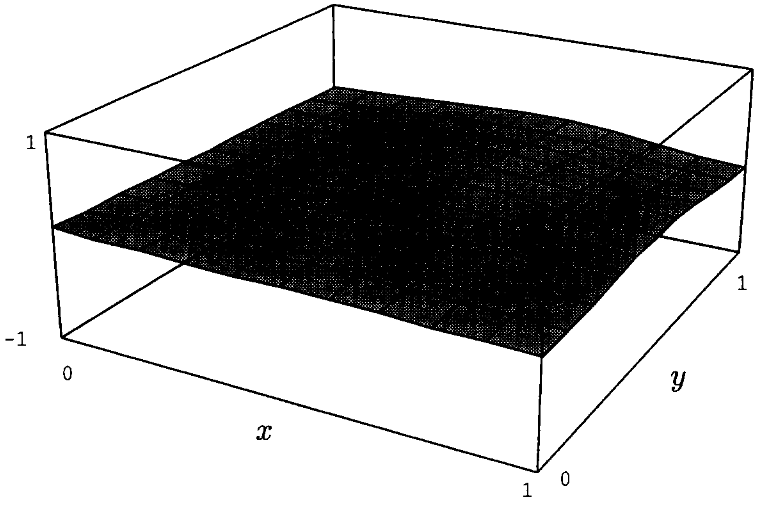

Figure 14. U^n at $t = 0.1$.

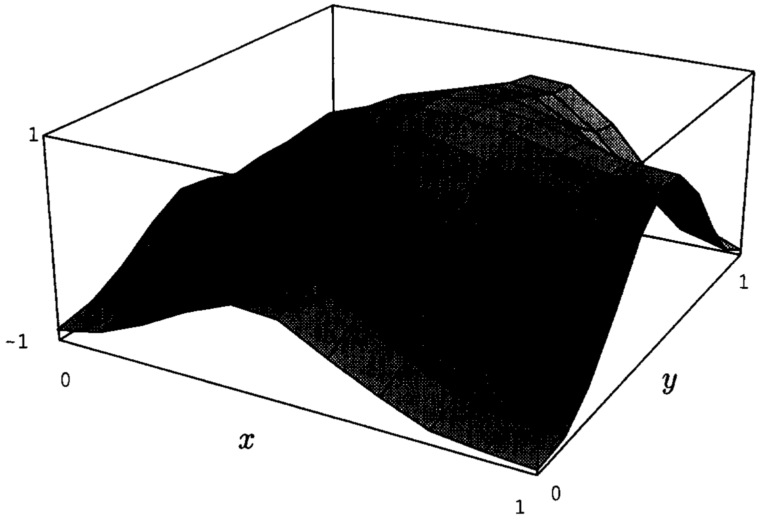

Figure 15. U^n at $t = 0.5$.

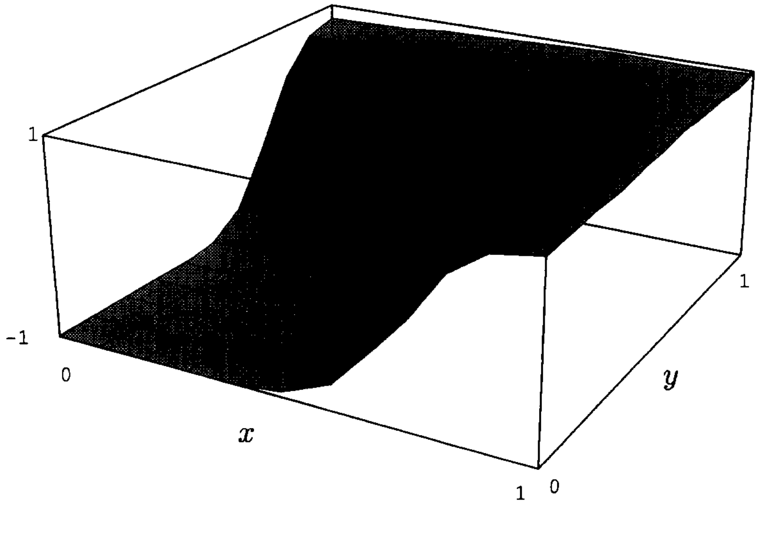

Figure 16. U^n at $t = 5.0$.

Figure 17. Total mass $f(t_n)$.

by the authors for the one-dimensional Cahn-Hilliard equation. Qualitative properties of the nonlinear finite difference scheme are analyzed as well as numerical computations. The nonlinear finite difference scheme is unconditionally stable and of a second order of accuracy. Several numerical examples are given, which show that the numerical solutions are physically meaningful. Comparison of the nonlinear scheme to the linearized scheme proposed by Sun [10] are given. Unlike in the linearized scheme, the nonlinear scheme can be applied to the problem with nonsmooth initial data and preserves the total mass. Even though the proposed finite difference method has the same order of convergence with those obtained by finite element methods (see [6,9]), it has some advantages in computational implementation.

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